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Using tools developed within the context of quantum information theory, we study the relaxation of a quantum system towards the thermal equilibrium. A two-qubit machine $U$ is called a *thermalizing machine* if (1) for all input state of the system $\rho$, after a sufficiently large number $n$ of interactions with the bath the system approaches the equilibrium state, and (2) the equilibrium state is stable. We characterize all the thermalizing machines, in particular by deriving a fluctuation-dissipation theorem, and by calculating the amount of entanglement that they can generate. The interplay of quantum and classical information processes that give rise to irreversibility is discussed.

The hypothesis of the quantum appeared suddenly in physics as an offspring of thermodynamics, due to the work of Planck on the blackbody radiation. In its early days however, the new theory developed rather as a form of mechanics, with a *reversible dynamics*. One century after Planck's intuition, the link between quantum mechanics (QM) and thermodynamics has been discussed by several scientists, and is still an actual field of research [1]. In parallel to fundamental issues, the concept of *quantum machines* has arisen recently in the field of quantum information processing [2]. Looking back again to history, we see that thermodynamics was born to describe engines. It is thus natural to ask whether there is a "thermodynamics" of quantum machines, and whether the modern standpoint of quantum information can cast some new light on the foundations of thermodynamics.

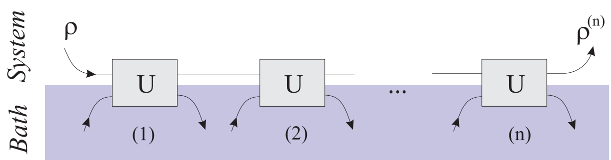


FIG. 1. The quantum channel: a repeated application of a unitary $U$ (quantum machine) that couples the state of the system with the state of the bath.

A typical problem of thermodynamics is the problem of *thermalization*, that is, the description of the relaxation towards the thermal equilibrium by a system in contact with a huge reservoir (bath). If one thinks of thermalization in terms of quantum machines and quantum information, a natural model is the following. The quantum system passes through several identical machines $U$ (figure 1), or several time through the same machine; at each passage, it becomes entangled (that is, it shares a part of the information encoded in the state) with an ancilla. At the output of the machine, the ancilla is discarded into the bath [3]: the information present in the system has undergone some degradation, that depends on the state of the bath and on the machine. Such a model for thermalization is known as a *collision model*, since the system becomes thermalized through interactions with the bath that are localized in time. Several general results on this thermalization problem have been obtained [4]. Thermalization through repeated collisions provides also the way to simulate the approach to thermal equilibrium with a quantum computer, as noticed recently by Terhal and DiVincenzo [5].

The rigorous definition of the thermalization problem involves two requirements: Let $\rho_B$ is the state of the bath, $\rho$ is a generic state of the system, $\rho^{(n)}$ is the state of the system after $n$ collisions (interactions with the machine), and, finally, $\rho^e$ is the state of the system at thermal equilibrium. The conditions we impose read:
*Requirement 1:* the state $\rho^e \otimes \rho_B$ is stationary under the application of the quantum machine $U$.
*Requirement 2:* If the system is prepared in a state $\rho \neq \rho^e$, we want the iteration of $U$ to lead finally to the equilibrium state, i.e. $\rho^{(n)} \rightarrow \rho^e$.

The key question we address in this Letter is: Which are (if any) the *thermalizing quantum machines*, i.e. the machines that thermalize a quantum system via an interaction with ancillas extracted from a thermal bath? In what follows we give the complete characterization of these machines in the case where both the system and the ancillas are qubits. Having characterized the whole family of thermalizing machines, we discuss first some thermodynamical issues; in particular, we can define the dissipation through a fluctuation-dissipation (FD) theorem. Then we provide an analysis of these machines using concepts that come from quantum information theory.

We start with a description of the model:
(i) The system is considered to be a qubit.
(ii) The bath is a reservoir composed of $N$ qubits; as usual in the studies of thermalization, we suppose that the number $N$ of qubits in the bath is infinite for any practical purpose. Each qubit in the bath is in an eigenstate of the one-qubit Hamiltonian $h = -\frac{E}{2}\sigma_z = \frac{E}{2}(P_1 - P_0)$, with $P_0 = |0\rangle\langle 0|$, $P_1 = |1\rangle\langle 1|$, and $E > 0$. The state of the bath can then be written $\rho_B = (\xi)^{\otimes N}$ with

$$\xi \; = \; pP_0 + qP_1 \; , \; q = 1 - p \, . \qquad (1)$$

The weight $p$ is linked to the temperature $\beta = 1/kT$ through $p = \frac{1}{2}(1 + \tanh \beta \frac{E}{2})$; in particular, $p = 1$ corresponds to a zero temperature, while $p = \frac{1}{2}$ is associated with the infinite temperature.

(iii) The machine $U$ is a unitary operation on $\mathbb{C}^2 \otimes \mathbb{C}^2$. This means that at each collision the system interacts with just a *single* qubit taken out of the bath. The fact that the bath is "infinite" guarantees that a qubit of the bath undergoes at most one collision with the system; therefore the input state of the ancilla is always $\xi$, and we write

$$\rho^{(k+1)} = \mathrm{Tr}_B\big[U\,(\rho^{(k)} \otimes \xi)\,U^\dagger\big] \;\equiv\; T_\xi\,[\rho^{(k)}]\,, \tag{2}$$

where $\mathrm{Tr}_B$ is the partial trace over the bath's qubit. In the case of the model under consideration the two requirements 1 and 2 read:

$$\text{Req. 1:}\;\; U\,(\xi \otimes \xi)\,U^\dagger = \xi \otimes \xi \;\;,\, \xi = pP_0 + qP_1 \;,\forall\, p \tag{3}$$

$$\text{Req. 2:}\;\; \rho^{(n)} = T_\xi^n[\rho] \;\longrightarrow \xi \;\;\forall\, \rho \tag{4}$$

Now, we specify the family of machines $U$ that meet these requirements. The condition (3) implies that the subspaces $P_0 \otimes P_0$, $P_1 \otimes P_1$ and $P_0 \otimes P_1 + P_1 \otimes P_0$ must be invariant under the action of $U$. In fact, $U\,P_0 \otimes P_0\,U^\dagger$ appears with the weight $p^2$, $U\,\big(P_0 \otimes P_1 + P_1 \otimes P_0\big)\,U^\dagger$ with the weight $p(1-p)$, and $U\,P_1 \otimes P_1\,U^\dagger$ with the weight $(1-p)^2$. Since we want condition (3) to hold for all $p$, the three subspaces must be separately invariant [6]. Consequently, up to a global phase factor, all unitary operations that fulfill the condition (3) are of the form

$$\begin{array}{rcl} U|0\rangle|0\rangle &=& |0\rangle|0\rangle\,;\\ U|1\rangle|1\rangle &=& e^{i\gamma}|1\rangle|1\rangle\,;\\ U|0\rangle|1\rangle &=& e^{i\theta}\big(\cos\phi|0\rangle|1\rangle + e^{i\chi}\sin\phi|1\rangle|0\rangle\big)\,;\\ U|1\rangle|0\rangle &=& e^{i\theta'}\big(e^{i\chi}\cos\phi|1\rangle|0\rangle - \sin\phi|0\rangle|1\rangle\big)\,, \end{array} \tag{5}$$

where $\phi \in [0, \frac{\pi}{2}]$. In summary: once the eigenstates of individual bath qubits $|0\rangle$ and $|1\rangle$ are fixed (e.g., eigenstates of the free Hamiltonian), the Requirement 1 is satisfied for all $p$ if and only if $U$ belongs to the five-parameters family of transformations specified by Eq. (5). In this family, we have to determine those $U$ that satisfy the Requirement 2 as well.

In what follows we explicitly present the iteration of the completely positive map $T_\xi$ generated by $U$. Let the initial state of the system be

$$\rho = d\,P_0 \,+\, (1-d)\,P_1 \,+\, k|0\rangle\langle 1| \,+\, k^*|1\rangle\langle 0|\,, \tag{6}$$

with $|k| \le \sqrt{d(1-d)}$, with equality if and only if $\rho$ is a pure state. Using the explicit form (5) for $U$, we find that $\rho^{(1)} = T_\xi[\rho] = d'\,P_0 \,+\, (1-d')\,P_1 \,+\, k'|0\rangle\langle 1| \,+\, k'^*|1\rangle\langle 0|$ with

$$d' \,=\, p\sin^2\phi + d\cos^2\phi \;\;,\;\; k' \,=\, \cos\phi\, k\,(re^{i\lambda})\,, \tag{7}$$

where $re^{i\lambda} = \big(pe^{-i(\chi+\theta')} + qe^{i(\theta-\gamma)}\big)$. Note that $r = \big[1 - 4pq\sin^2(\frac{\theta+\theta'+\chi-\gamma}{2})\big]^{\frac{1}{2}} \le 1$. The effect of the map on both the diagonal term $d$ and the off-diagonal term $k$ can be iterated straightforwardly, and we find after $n$ iterations

$$d^{(n)} = (1-(\cos\phi)^{2n})\,p \,+\, (\cos\phi)^{2n}\,d\,, \tag{8}$$

$$k^{(n)} = k\,\big(r\,\cos\phi\big)^n e^{i\lambda n}\,. \tag{9}$$

Thus, whenever $\cos\phi < 1$, the iteration of $T_\xi$ yields $d^{(n)} \to p$ and $k^{(n)} \to 0$, that is, $\rho^{(n)} \to \xi$: almost all the machines of the form (5) satisfy Requirement 2.

Let us briefly consider the case $\cos\phi = 1$. In this case $d^{(n)} = d$ for all $n$; but still $k^{(n)} \to 0$, unless $r = 1$ i.e. $\theta + \theta' + \chi - \gamma = 0$. So $\rho^{(n)} \to dP_0 + (1-d)P_1$: the iteration of $T_\xi$ does not converge to the state of the bath $\xi$, but to the outcome of the von Neumann measurement in the basis of the eigenstates of the bath (all states of the form $xP_0 + (1-x)P_1$ are fixed points of $T_\xi$).

Having the complete family of thermalizing machines (5), we proceed to study their properties, first in terms of thermodynamics, then from the standpoint of quantum information.

*Energy conservation.* The family of unitary operations given by Eq. (5) has an immediate physical meaning. For the sake of the argument, imagine that all our qubits (the system and the bath) are spins in a uniform magnetic field. In our model, all these spins are non-interacting, except during the collisions $U$ that thermalize the system; thus between two collisions the Hamiltonian is simply $H = \sum_i h[i]$, with $h[i] = \frac{E}{2}(P_1^{(i)} - P_0^{(i)})$ being the one-qubit Hamiltonian $h$ acting on the $i$-th qubit. If the collision is described by Eq. (5), then only $|0\rangle|1\rangle$ and $|1\rangle|0\rangle$ become superposed. Obviously, with respect to the Hamiltonian $H$ these states are degenerate. In other words, the interactions $U$ commutes with the Hamiltonian $H$, i.e. $[U, H] = 0$. Consequently, the energy of interaction with an external field is conserved through the collision. Thus, the thermalizing $U$ are those that ensure energy conservation.

*Relaxation times.* We would like to pass from an interaction through discrete collisions to an interaction continuous in the time parameter $t$. This is possible because $U \to \mathbb{1}$ when the parameters $\phi$, $\gamma$, $\theta$, $\theta'$ and $\chi$ go to 0. In the continuous-time limit, the iteration (8) for $d^{(n)}$ and the iteration (9) for $k^{(n)}$ can be written using the usual definition of the relaxation times $T_1$ and $T_2$ [8]:

$$d(t) = e^{-t/T_1}d(0) + (1 - e^{-t/T_1})p\,, \tag{10}$$

$$|k|(t) = e^{-t/T_2}|k|(0)\,. \tag{11}$$

To perform the limit, we set $n = t/\tau_0$, and we let the interaction time $\tau_0 \to 0$ together with the parameters defining $U$. We have

$$(\cos^2\phi)^n \approx (1-\phi^2)^{\frac{t}{\tau_0}} \;\longrightarrow\; e^{-\frac{\phi^2}{\tau_0}\,t} \tag{12}$$

in the limit $\tau_0 \to 0$, with $\frac{\phi^2}{\tau_0} = \frac{1}{T_1}$ constant. Similarly, writing $x = pq(\theta + \theta' + \chi - \gamma)^2$, we have

$$(r\,\cos\phi)^n \approx \big(1 - (x+\phi^2)/2\big)^{\frac{t}{\tau_0}} \;\longrightarrow\; e^{-\frac{x+\phi^2}{2\tau_0}\,t} \tag{13}$$

with $\frac{x}{\tau_0}$ constant. We have the freedom to choose either $T_1$ or $T_2$, because $\tau_0$ is defined up to a multiplicative constant; but the two relaxation rates are related as

$$\frac{1}{T_2} = \frac{1}{2\,T_1}\left(1 + p\,q\,\frac{(\theta+\theta'+\chi-\gamma)^2}{\phi^2}\right). \tag{14}$$

Note that, in general, the ratio $\frac{T_1}{T_2}$ depends on the temperature. For some $U$, the bound $T_1 \geq \frac{1}{2}T_2$ (see e.g. [4], p. 120) is saturated.

*Fluctuation-dissipation (FD) theorem.* A FD theorem links the fluctuations at equilibrium and the mechanisms of dissipation. We have seen above that dissipation is essentially characterized by the parameter $\phi$: the higher this parameter, the faster equilibrium is reached. In this paragraph, we introduce a measure of fluctuations and see how it depends on $\phi$. To quantify the fluctuations, we consider the following protocol. First, the system is prepared in the equilibrium state $\xi$ and is measured in the basis of its eigenstates $P_0$ and $P_1$. Obviously, the mean values of one-qubit observables $A$ are unaffected by this measurement. Then we let the system to undergo $n$ interactions with the bath qubits: from the state $P_j$ $(j=0,1)$ in which it had been found by the measurement, the system evolves into the state $\rho_j^{(n)} = T_\xi^n[P_j]$. By the definition of equilibrium, $p\rho_0^{(n)} + q\rho_1^{(n)} = \xi$; in particular, the mean value of $A$ holds unchanged. However, due to the information gained through the measurement, now we have also access to the following statistical quantity:

$$F_A^{(n)} = \sqrt{p\big[\mathrm{Tr}(\delta_0^{(n)}\,A)\big]^2 + q\big[\mathrm{Tr}(\delta_1^{(n)}\,A)\big]^2}\,, \tag{15}$$

where $\delta_j^{(n)} = \rho_j^{(n)} - P_j$ is the deviation from the measured state $P_j$ after $n$ interactions. $F_A^{(n)}$ is a measure of the fluctuations of $A$; the dissipative element can be seen through the fact that if $F_A^{(n)} \neq 0$, then the fluctuations have partly erased the information that we had obtained through the measurement. Using (8) we find $\delta_0^{(n)} = -q(1-(\cos\phi)^{2n})\sigma_z$ and $\delta_1^{(n)} = p(1-(\cos\phi)^{2n})\sigma_z$, whence writing $D^{(n)} = (1-(\cos\phi)^{2n})$ we find

$$F_A^{(n)} = D^{(n)}\,\frac{1}{2\,\cosh(\beta E/2)}\,\big|\mathrm{Tr}(A\sigma_z)\big|\,. \tag{16}$$

In the continuous time limit, $D^{(n)}$ is replaced by $D(t) = (1-e^{-t/T_1})$. This is our FD theorem: the fluctuations $F$ are proportional to the dissipation $D$ through a function of the temperature. The fluctuations are absent at zero temperature, while they are maximal at infinite temperature. Usually one considers the fluctuations of the one-qubit hamiltonian $h$, in which case $|\mathrm{Tr}(h\sigma_z)| = E$ the splitting of the energy levels.

*Information conservation.* We begin the analysis of the thermalizing machines in terms of information with some general considerations. After the system qubit is thermalized, it is in the same state as the bath qubits are. This does not mean that the information encoded in the initial state of the system $\rho$ is lost: indeed, since we considered only unitary transformations, the information is encoded in a different way, being spread between the system and the bath. But one cannot retrieve this information, unless one knows which qubits of the bath have undergone a collision with the system, and in which order. Here, thermodynamical irreversibility (dissipation) arises as the interplay of two information processes: (i) the *quantum information* on the initial state of the system is spread between the system and the bath, still in a reversible way; (ii) the *classical information* about the order of the collisions is lost, leading to the practical impossibility of running the process backwards. As an application, one can define "safes" for quantum information that can be "opened" with classical keys [7].

*Link with known quantum machines.* To our knowledge, only one among the thermalizing machines (5) had already been discussed within the context of quantum information processing. A machine whose action is $U|00\rangle = |00\rangle$, $U|10\rangle = \cos\phi|10\rangle + \sin\phi|01\rangle$ is a particular realization of the two-qubit copying machine proposed by Niu and Griffiths [9]. In quantum cryptography, this machine defines Eve's optimal individual attack on the four-state protocol.

*The partial swap.* In the five-parameters family of the thermalization transformations (5), a particular role is played by the specific one-parameter family:

$$\begin{aligned}
V(\phi)|0\rangle|0\rangle &= |0\rangle|0\rangle\,;\\
V(\phi)|1\rangle|1\rangle &= |1\rangle|1\rangle\,;\\
V(\phi)|0\rangle|1\rangle &= e^{-i\phi}\big(\cos\phi|0\rangle|1\rangle + i\sin\phi|1\rangle|0\rangle\big)\,;\\
V(\phi)|1\rangle|0\rangle &= e^{-i\phi}\big(\cos\phi|1\rangle|0\rangle + i\sin\phi|0\rangle|1\rangle\big)\,.
\end{aligned} \tag{17}$$

We call this machine the *partial swap* [7], since

$$V(\phi) = e^{-i\phi}\left(\cos\phi\,\mathbb{1} + i\sin\phi\,U_{sw}\right) = e^{-i\frac{\phi}{2}}\,e^{i\frac{\phi}{2}\vec{\sigma}\otimes\vec{\sigma}}\,, \tag{18}$$

where $U_{sw} = V(\frac{\pi}{2})$ is the swap operation, i.e. it is the unitary operation whose action is $|\psi_1\rangle\otimes|\psi_2\rangle \longrightarrow |\psi_2\rangle\otimes|\psi_1\rangle$ for all $|\psi_1\rangle\,,\,|\psi_2\rangle \in \mathbb{C}^2$. Note that the swap is the most trivial and the fastest way to achieve thermalization in a collision model: from the very first collision, the state of the system is "lost" into the bath, and one of the qubits of the bath becomes the system. Thus, the partial swap conveys the intuitive idea, that at each collision part of the information contained in the state of the system is transferred into the bath.

The family of partial swaps has a remarkable property. These machines satisfy Requirements 1 and 2 *for all states* $\xi$; it can be shown that *only* the partial swaps have this property [7]. Using again the image of the spins in the magnetic field, this means that this $U$ leads to thermalization whatever the direction of the magnetic field. More generally, it is possible to use the partial swaps to define a new process that we call *homogenization.* Consider a reservoir containing a finite number of qubits in an arbitrary but fixed state $\xi$. Unlike thermalization, the homogenization process does not single out any priviledged basis. Applying the partial swap $n$ times, just as in fig. 1, the state of the system ends up in some vicinity of the state $\xi$. At the end of the process, every qubit is approximately in the state $\xi$: the system qubit and the bath qubits undergo a mutual homogenization. This process is more similar to typical quantum information processes, like cloning. For more details on homogenization, see Ref. [7].

*Creation of Entanglement.* In general, the thermalizing machines (5) entangle the system with the bath. In the context of quantum information, the generation of entanglement by non-local unitary operations has been the object of recent investigation [10–12]. Kraus and Cirac [11] showed that any unitary operation on two qubits can be decomposed as $U = (u_A \otimes u_B)\, e^{iH_d}\, (v_A \otimes v_B)$, where $H_d = \sum_{i=x,y,z} a_i \sigma_i \otimes \sigma_i$, and the $u$'s and the $v$'s are one-qubit unitary operations. Thus the entanglement generated by $U$ depends only on $H_d$. For the thermalizing machines $U$ given by Eq. (5) we find the following decomposition:

$$U(\phi, ...) = [u(\alpha') \otimes u(\beta')]\, V(\phi)\, [u(\alpha) \otimes u(\beta)]\,, \qquad (19)$$

where $V(\phi)$ is the partial swap and $u(x) = P_0 + e^{ix} P_1$ [14]; the other parameters are given by $\gamma = \alpha + \beta + \alpha' + \beta'$, $\theta = \beta + \beta' - \phi$, $\theta' = \alpha + \beta' - \phi - \frac{\pi}{2}$, $\chi = \alpha' - \beta' + \frac{\pi}{2}$. The partial swap is thus at the heart of all thermalizing machines.

Let now $C(|\Psi\rangle) = \left|\langle\Psi|\sigma_y \otimes \sigma_y|\Psi^*\rangle\right|$ be the measure of entanglement known as concurrence [13]. The *entangling power* of $U$ can be defined either as the average $C_{av}$ [10], or as the maximum $C_{max}$ [11], of $C(|\Psi\rangle)$ over all $|\Psi\rangle = U|\psi_1\rangle \otimes |\psi_2\rangle$. Since the partial swap is invariant under bilateral rotation, we can calculate the concurrence for states of the form $|\Psi_{a,b}\rangle = V(\phi)|0\rangle \otimes (a|0\rangle + b|1\rangle)$. The result is $C(|\Psi_{a,b}\rangle) = |b|^2 \sin 2\phi$. Therefore $C_{max} = \sin 2\phi$ and (supposing that the average is calculated using the uniform measure on the sphere) $C_{av} = \frac{\pi}{4} \sin 2\phi$.

*Entanglement and Dissipation.* Both the dissipation $D^{(n)} = (1 - (\cos\phi)^{2n})$ and the entangling power $C \propto \sin 2\phi$ are determined by $\phi$. The behavior of $D$ and $C$ is globally different: $D$ is maximum for $\phi = \frac{\pi}{2}$, that is for the swap (thermalization in one step); while $C$ is maximum for $\phi = \frac{\pi}{4}$, and falls to zero for the swap. However, a swap is not a good model for thermalization in the physical world [3]: thermalization means to have the system undergo many small interactions with the reservoir, rather than to take the state of the system and throw it in a universal dustbin. In this sense, physical thermalization is obtained in the limit $\phi \to 0$, and in this limit $D \propto C^2 \propto \phi^2$. In other words: entanglement and dissipation are not identical, since entanglement measures the *sharing* of the quantum information between the system and the bath, while dissipation measures the rate of *transfer* of quantum information from the system to the bath. However, for small interactions one can transfer the information on the system into some correlations. Clearly, the link between entanglement and dissipation deserves further investigation.

The analogy between quantum information and thermodynamics has been studied under different perspectives in the last years [15]. In this Letter, we investigated this analogy by examining the role of quantum information concepts, like entanglement, in the process of thermalization. We acknowledge fruitful discussions with Ignacio Cirac, Mark Hillery, Günther Mahler and Sandu Popescu. Part of this work was prepared during the ESF Conference on Quantum Information (Gdańsk, 10-18 July 2001). This was work partially supported by the European Union project EQUIP (IST-1999-11053).

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